

# Nonlinear higher-order hydrodynamics. Unification of kinetic and hydrodynamic approaches within a nonequilibrium statistical ensemble formalism.

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## Abstract

Construction, in the framework of a Nonequilibrium Statistical Ensemble Formalism, of a Mesoscopic Hydro-Thermodynamics, that is, covering phenomena involving motion displaying variations short in space and fast in time –unrestricted values of Knudsen numbers–, is presented. In that way, it is provided an approach enabling for the coupling and simultaneous treatment of the kinetics and hydrodynamic levels of descriptions. It is based on a complete thermo-statistical approach in terms of the densities of matter and energy and their fluxes of all orders covering systems arbitrarily driven away from equilibrium. The set of coupled nonlinear integro-differential hydrodynamic equations is derived. They are the evolution equations of the Grad-like moments of all orders, derived from a generalized kinetic equation built in the framework of the Nonequilibrium Statistical Ensemble Formalism. For illustration, the case of a system of particles embedded in a fluid acting as a thermal bath is fully described. The resulting enormous set of coupled evolution equations is of unmanageable proportions, thus requiring in practice to introduce an appropriate description using the smallest possible number of variables. We have obtained a hierarchy of Maxwell times, which can be considered a kind of Bogoliubov's characteristic times in hydrodynamic and which have a particular relevance in the criteria for establishing a contraction of description.

## I. INTRODUCTION

It has been noticed that one of the complicated problems of the nonequilibrium theory

of transport processes in dense gases and liquids is the fact that their kinetics and hydro-

dynamics are intimately coupled, and must be treated simultaneously (e.g., see Refs. [1]-[6]). On this we may say that microscopic descriptions of hydrodynamics, that is, associated to a derivation of kinetic equations from classical or quantum mechanics and containing kinetic (transport) coefficients written in terms of correlation functions, is a long standing traditional problem. An important aspect is the derivation of constitutive laws which express thermodynamic fluxes (or currents, as those of matter and energy) in terms of appropriate thermodynamic forces (typically gradients of densities as those of matter and energy). In their most general form these laws are nonlocal in space and non-instantaneous in time. A first kinetic-hydrodynamic approach can be considered to be the so-called *classical (or Onsagerian) hydrodynamics*; it gives foundations to, for example, the classical Fourier's and Fick's diffusion laws. But it works under quite restrictive conditions, namely, local equilibrium; linear relations between fluxes and thermodynamic forces (meaning weak amplitudes in the motion) with Onsager's symmetry laws holding; near homogeneous and static movement (meaning that the motion can be well described with basically Fourier components with long wavelengths and low frequencies, and then involves only smooth variation in space and time); weak and rapidly regressing

fluctuations [3]-[7].

Hence, more advanced approaches are required to lift these restrictions. Consider first near homogeneity, which implies validity in the limit of long wavelengths (or wavenumber  $Q$  approaching zero). To go beyond it is necessary to introduce a proper dependence on  $Q$  valid, in principle, for intermediate and short wavelengths (intermediate to large wavenumbers). In phenomenological theories this corresponds to go from classical irreversible thermodynamics to extended irreversible thermodynamics [8]-[10]. This is what has been called *generalized hydrodynamics*, a question extensively debated for decades by the Statistical Mechanics community. Several approaches have been used, and a description can be consulted in Chapter 6 of the classical book on the subject by Boon and Yip [2]. Introduction of non-local effects for describing motions with influence of ever decreasing wavelengths, going towards the very short limit, has been done in terms of expansions in increasing powers of the wavenumber, which consists in what is sometimes referred to as *higher-order hydrodynamics* (HOH). Attempts to perform such expansions are the so-called Burnett and super-Burnett approaches in the case of mass motion, and Guyer-Krumhansl approach in the case of propagation of energy (see for example Refs. [11] and [12]).

An usual approach has been based on the moments solution procedure of Boltzmann equation, as in the work of Hess [13], using a higher-order Chapman-Enskog solution method. The Chapman-Enskog method provides a solution to Boltzmann equation consisting of a series in powers of the Knudsen number,  $K_n$ , given by the ratio between the mean-free path of the particles and the scale of change (relevant wavelengths in the motion) of the hydrodynamic fields. Retaining the term linear in  $K_n$  there follows Navier-Stokes equation, the term in  $K_n^2$  introduces Burnett-like contributions, and the higher-order ones ( $K_n^3$  and up) the super-Burnett contributions.

A satisfactory development of a HOH being also nonlinear and including fluctuations is highly desirable for covering a large class of hydrodynamic situations, and, besides its own scientific interest, also for obtaining insights into present day technological-industrial processes. Also, we can mention its fundamental relevance in Oceanography and Meteorology (e.g. [14], [15]), and that it has been stated [16] that the idea of promoting hydraulics by statistical inference is appealing because the complete information about phenomena in hydraulics seldom exists; for example sediment transport and the more fundamental problem in fluid mechanics of describing the velocity distribution in flu-

ids under flow [17]-[19]. Indeed, the nonlocal terms become specially important in miniaturized devices at submicronic lengths [20], or in the design of stratospheric planes, which fly in rarefied gases in a density regime between the independent particle description and the purely continuous description. Another particular problem to it related is the one of obtaining the structures of shock waves in fluids for wide ranges of Mach numbers [21]. Moreover, Burnett approximation of hydrodynamics has been shown to provide substantial improvement on many features of the flow occurring in several problems in hydrodynamics, e.g. the case of Poiseuille flow [22] and others [23].

The microscopic derivation of a HOH, together with the analysis of the validity of existing theories, is still a point in question. It has been shown [24] that for the case of Maxwellian molecules, whereas Navier-Stokes approximation yields equations which are stable against small perturbations, this is not the case when are introduced Burnett contributions to the equations. It follows that small perturbations to the solutions, which are periodic in the space variable with a wavelength smaller than a critical length, are exponentially unstable. This fact has been called *Bobylev's instability*. Moreover, Karlin [25] reconsidered the question looking for exact solutions to simplified mod-

els: When a linearized ten-moments Grad method is used, and the Chapman-Enskog method is applied to the model, does in fact there follow instabilities in the higher-order approximations. On the other hand, resorting to the Chapman-Enskog solution for linearized Grad ten-moment equations resummed exactly, solutions are obtained for which the stability of higher-order hydrodynamics, in various approximations, can be discussed. However, more recently, Garcia-Colin and collaborators [26] have extended Bobylev's analysis for the case of any interaction potential, and have demonstrated that one can interpret the fact as to give a bound for a Knudsen number above which the Burnett equations are not valid, with no instability involved.

Furthermore, inclusion of nonlinearity in the theory, in a Mesoscopic Hydro-Thermodynamics (MHT for short and meaning thermal physics of fluid continua), leads to additional possible singularities, called hydrodynamic singularities, as, for example, those described in Refs. [27]-[29]. A satisfactory construction of a MHT is highly desirable for covering a large class of hydrodynamic situations obtaining an understanding of the physics involved from the microscopic level, and in the last instance gaining insights into technological and industrial processes as in, for instance, hydraulic engineering, food

engineering, soft-matter engineering, oil production and petrochemistry, etc., which have an associated economic interest. MHT was initiated by the so-called Catalan School of Thermodynamics as a large expansion of Extended Irreversible Thermodynamics [30].

It can be noticed that nowadays two approaches appear to be the most favorable for providing very satisfactory methods to deal with hydrodynamics within an ample scope of nonequilibrium conditions. They are Nonequilibrium Molecular Dynamics (NMD) [31] and the kinetic theory based on the far reaching generalization of Gibbs' ensemble formalism, namely the Nonequilibrium Statistical Ensemble Formalism (NESEF for short) [32]-[36]. NMD is a computational method created for modeling physical system at the microscopic level, being a good technique to study the molecular behavior of several physical processes. Together with the so-called Monte Carlo method are part of what is known as numeric simulation methods [37].

We do here present an extensive derivation of a MHT on the basis of the kinetic theory founded on NESEF, quite appropriate to deal with systems in far-from-equilibrium conditions involving the development of ultrafast relaxation processes, and displaying nonlinear behavior leading, eventually, to instabilities and synergetic self-organization [38]-[40]. Within the framework of NESEF, but in a

different approach to the one used here, an alternative MHT was introduced by Zubarev and Tishchenko [41], [42].

It may be noticed that the formalism can be extended to deal with the so-called non-conventional hydrodynamics which is associated to disordered media [43], consisting in systems showing a complex structure of a fractal-like (self-affine in average) characteristics, whose range of applicability and of physical interest is large [44]. Fall on this problem the case of the distinctive behavior of polyatomic structures such as colloidal particles, surfactant micelles, and polymer and biopolymer (as DNA) in liquid solutions, which are classical examples of what is presently referred to as soft condensed matter [45]. One particular case of apparently unusual behavior is the one associated to hydrodynamic motion leading to a so-called non-Fickian diffusion, described by a time evolution following a kind of fractional-power law [46]. The nonequilibrium statistical thermomechanical aspects of complex systems including illustrations is reported elsewhere [47]; a case involving hydro-thermodynamics is given in Ref. [48].

In the present paper the conventional NESEF-based MHT is described in next Section, accompanied with the study of a system consisting of particles embedded in a fluid which acts as a thermal bath at rest

and in thermal equilibrium with an external reservoir. The general theory for the MHT is built upon a generalization of Grad's moments method for solution of, in this case, a generalized kinetic equation derived in the context of NESEF [58].

## II. THEORETICAL BACKGROUND

For building a nonlinear higher-order (generalized) hydro-thermodynamics on mechanical statistical basis, one needs to resort to a nonequilibrium statistical ensemble formalism (NESEF) for open systems. Such formalism was developed step by step along the past century by a number of renowned scientists whose contributions have been systematized and generalized in a close structure, as described in Refs. [32] to [36].

According to theory, immediately after the open system of  $N$  particles, in contact with external sources and reservoirs, has been driven out of equilibrium, the description of its state requires to introduce all its observables, their fluctuations and, eventually, higher-order variances. In most cases it suffices to take a reduced set of observables, what implies in to have access to the so-called one-particle (or single-particle),  $\hat{n}_1$ , and two-particle,  $\hat{n}_2$ , dynamical operators for any subset of the particles involved. This is so because all observable quantities can be ex-

pressed at the microscopic mechanical level in terms of these operators (e.g. Refs. [49] and [50]).

On the basis of the construction of the nonequilibrium statistical operator [32]-[33], and taking into account the noted above fact that a complete description of the nonequilibrium state of the system follows from the knowledge of the single- and two-particle density operators (or equivalently the associated reduced density matrices) which in classical mechanics are

$$\hat{n}_1(\mathbf{r}, \mathbf{p}) = \sum_{j=1}^N \delta(\mathbf{r} - \mathbf{r}_j) \delta(\mathbf{p} - \mathbf{p}_j), \quad (1)$$

$$\begin{aligned} \hat{n}_2(\mathbf{r}, \mathbf{p}; \mathbf{r}', \mathbf{p}') &= \sum_{j \neq k=1}^N \delta(\mathbf{r} - \mathbf{r}_j) \delta(\mathbf{p} - \mathbf{p}_j) \\ &\times \delta(\mathbf{r}' - \mathbf{r}_k) \delta(\mathbf{p}' - \mathbf{p}_k), \end{aligned} \quad (2)$$

where  $\mathbf{r}_j, \mathbf{p}_j$  are the coordinate and momentum of the  $j$ -th particle, and  $\mathbf{r}, \mathbf{p}$  are called field variables, the most complete nonequilibrium statistical distribution [4], [32]-[36] is the one built in terms of the auxiliary statistical operator

$$\bar{\mathcal{R}}(t, 0) = \bar{\rho}(t, 0) \times \rho_R, \quad (3)$$

where  $\bar{\rho}$  refers to the system of  $N$  particles of mass  $m$ , and  $\rho_R$  is the one associated to a thermal bath of  $N_R$  particles of mass  $M$  taken in equilibrium at temperature  $T_0$ . The first one is given by

$$\bar{\rho}(t, 0) = \exp \left\{ -\phi(t) - \int d^3r d^3p F_1(\mathbf{r}, \mathbf{p}; t) \right.$$

$$\begin{aligned} &\times \hat{n}_1(\mathbf{r}, \mathbf{p}) \\ &- \int d^3r d^3p \int d^3r' d^3p' F_2(\mathbf{r}, \mathbf{p}, \mathbf{r}', \mathbf{p}'; t) \\ &\times \hat{n}_2(\mathbf{r}, \mathbf{p}, \mathbf{r}', \mathbf{p}') \left. \right\}. \end{aligned} \quad (4)$$

Hence,  $\bar{\rho}(t, 0)$  depends on the variables of the system of interest and  $\rho_R$  on the variables of the thermal bath; both distributions are taken as normalized, as it should, with  $\phi(t)$  ensuring the normalization of  $\bar{\rho}$ , that is,

$$\begin{aligned} \phi(t) &= \int d\Gamma \exp \left\{ - \int d^3r d^3p F_1(\mathbf{r}, \mathbf{p}; t) \right. \\ &\times \hat{n}_1(\mathbf{r}, \mathbf{p}) \\ &- \int d^3r d^3p \int d^3r' d^3p' F_2(\mathbf{r}, \mathbf{p}, \mathbf{r}', \mathbf{p}'; t) \\ &\times \hat{n}_2(\mathbf{r}, \mathbf{p}, \mathbf{r}', \mathbf{p}') \left. \right\}, \end{aligned} \quad (5)$$

and  $F_1$  and  $F_2$  are the nonequilibrium thermodynamic variables conjugated to  $\hat{n}_1$  and  $\hat{n}_2$  meaning that

$$\frac{\delta \ln \bar{\mathcal{Z}}(t)}{\delta F_1(\mathbf{r}, \mathbf{p}; t)} = -Tr \{ \hat{n}_1(\mathbf{r}, \mathbf{p}) \bar{\rho}(t, 0) \}, \quad (6)$$

$$\frac{\delta \ln \bar{\mathcal{Z}}(t)}{\delta F_2(\mathbf{r}, \mathbf{p}, \mathbf{r}', \mathbf{p}'; t)} = -Tr \{ \hat{n}_2(\mathbf{r}, \mathbf{p}; \mathbf{r}', \mathbf{p}') \bar{\rho}(t, 0) \}, \quad (7)$$

where  $\ln \bar{\mathcal{Z}}(t) = \phi(t)$  with  $\bar{\mathcal{Z}}(t)$  playing the role of a nonequilibrium partition function and  $\delta$  stands for functional derivative, in complete analogy with the equilibrium case. Moreover,  $d\Gamma$  is the element of volume in the phase space of the system, and for simplicity

we have omitted to indicate the dependence on  $\Gamma$  of  $\hat{n}_1$ ,  $\hat{n}_2$ ,  $\bar{\rho}$ ,  $\bar{\mathcal{R}}$ , and that  $\rho_R$  depends on the phase point  $\Gamma_R$  in the phase space of the bath.

We stress that  $\bar{\rho}$  of Eq.(4) is not the statistical operator of the nonequilibrium system, but an auxiliary one – called the “instantaneously frozen quasi-equilibrium” statistical operator – that allows to build the proper nonequilibrium statistical operator, which needs to include *historicity and irreversibility* not present in  $\bar{\rho}$ , hence it does not account for dissipative processes, and besides does not provide correct average values in the calculation of transport coefficients and response functions.

We recall that the nonequilibrium statistical operator is given by [4], [32]-[36]

$$\mathcal{R}_\varepsilon(t) = \exp \left\{ \ln \bar{\rho}(t, 0) - \int_{-\infty}^t dt' e^{\varepsilon(t'-t)} \frac{d}{dt'} \ln \bar{\rho}(t', t' - t) \right\} \times \rho_R, \quad (8)$$

with  $\bar{\rho}(t, 0)$  of Eq. (4), and where

$$\bar{\rho}(t', t' - t) = \exp \left\{ i(t - t') \mathcal{L} \right\} \bar{\rho}(t', 0), \quad (9)$$

is the auxiliary operator carrying on the mechanical evolution of the system under Hamiltonian  $\hat{H}$  ( $\mathcal{L}$  is the Liouvillian operator of the system meaning  $i\mathcal{L}\hat{A} = \{\hat{A}, \hat{H}\}$ ). Usually the system's Hamiltonian is separated out into two terms, namely,

$$\hat{H} = \hat{H}_0 + \hat{H}', \quad (10)$$

where  $\hat{H}_0$  is the kinetic energy operator and

$$\hat{H}' = \hat{H}_1 + \hat{W} + \hat{H}_P, \quad (11)$$

contains the internal interactions energy operator  $\hat{H}_1$ , while  $\hat{W}$  accounts for the interaction of the system with the thermal bath, and  $\hat{H}_P$  is the energy operator associated to the coupling of the system with external pumping sources. Finally,  $\varepsilon$  is an infinitesimal positive real number which is taken going to zero after the traces in the calculation of averages have been performed (it is present in a kernel that introduces irreversibility in the calculations, in a Krylov-Bogoliubov sense [32]-[34]). We stress that the second contribution in the exponent in Eq. (8) accounts for historicity and irreversible evolution from the initial time (taken in the remote past,  $t_0 \rightarrow -\infty$ , implying in adiabatic coupling of correlations, (see for example Ref. [32]), or alternatively, can be seen as the adiabatic coupling of the interactions responsible for relaxation processes [51]). Moreover we notice that the time derivative in Eq. (8) takes care of the change in time of the thermodynamic state of the system (the first term in the argument i.e.  $t'$ ) and of the microscopic mechanical evolution (second term in the argument, i.e.  $t' - t$ , see Eq. (9)), and that the

initial value condition is  $\mathcal{R}_\varepsilon(t_0) = \bar{\rho}(t_0, 0)$  for  $t_0 \rightarrow -\infty$ .

The nonequilibrium thermodynamic space of states [52] associated to the basic dynamic variables  $\hat{n}_1$  and  $\hat{n}_2$  is composed by the one-particle and two-particle distribution functions

$$\begin{aligned} f_1(\mathbf{r}, \mathbf{p}; t) &= Tr \{ \hat{n}_1(\mathbf{r}, \mathbf{p}) \varrho_\varepsilon(t) \} \\ &= Tr \{ \hat{n}_1(\mathbf{r}, \mathbf{p}) \bar{\varrho}(t, 0) \} \end{aligned} \quad (12)$$

$$\begin{aligned} f_2(\mathbf{r}, \mathbf{p}, \mathbf{r}', \mathbf{p}'; t) &= Tr \{ \hat{n}_2(\mathbf{r}, \mathbf{p}, \mathbf{r}', \mathbf{p}') \varrho_\varepsilon(t) \} \\ &= Tr \{ \hat{n}_2(\mathbf{r}, \mathbf{p}, \mathbf{r}', \mathbf{p}') \bar{\varrho}(t, 0) \} \end{aligned} \quad (13)$$

where we indicate that for the basic variables, and only for them, the average with the statistical operator  $\varrho_\varepsilon$  is equal to the one taken with the auxiliary operator [32]-[34]. The trace operation  $Tr$  is in this classical approach to be understood as an integration over phase space;  $\hat{n}_1$  and  $\hat{n}_2$  are functions on phase space and  $\bar{\varrho}$  and  $\varrho_\varepsilon$  functionals of these two. The knowledge of the two distribution functions  $f_1$  and  $f_2$  allows to determine the value and evolution of any observable of the system as well as of response functions and transport coefficients.

The knowledge of  $f_1(\mathbf{r}, \mathbf{p}; t)$  implies complete information about the actual distribution of particles, and therefore of the physical properties of the system. Alternatively, knowing all the moments of the distribution

allows to have a complete knowledge of its characteristics. A knowledge of some moments is not sufficient to determine the distribution completely; it implies in only possessing partial knowledge of the characteristics of this distribution [61]. Grad noticed that the question of the general solutions of the standard Boltzmann equation can be tackled along two distinct lines. One is to attempt to solve Boltzmann equation for the distribution  $f_1$  itself in specific problems. Other is to obtain new phenomenological equations in an approach initiated by Maxwell [63] and continued by Grad [[64], [66]] (it was called Grad's moments procedure [65]). These moments produce quantities with a clear physical meaning, namely, the densities of particles and of energy and the fluxes of particles of first and second order in a restricted fourteen-moments approach.

In brief, the  $r$ th-order moment is the flux of order  $r$

$$\mathbf{I}_s^{[r]}(\mathbf{r}, t) = \int d^3p u_s^{[r]}(\mathbf{p}) f_1(\mathbf{r}, \mathbf{p}; t) \quad (14)$$

where  $u_s^{[r]}$  is the  $r$ -rank tensor,  $s \equiv n$  for particle motion and  $s \equiv h$  for energy motion,

$$u_n^{[r]}(\mathbf{p}) = \left[ \frac{\mathbf{p}}{m} \dots (r - \text{times}) \dots \frac{\mathbf{p}}{m} \right], \quad (15)$$

$$u_h^{[r]}(\mathbf{p}) = \frac{p^2}{2m} u_n^{[r]}(\mathbf{p}),$$

that is, the tensorial product of  $r$ -times the vector  $\mathbf{p}/m$ ; for  $s \equiv n$ ,  $r = 0$  stands for the



density,  $r = 1$  for the vector flux (or current),  $r = 2$  for the flux of the flux which is related to the pressure tensor field, and  $r > 2$  for all the other higher-order fluxes. For  $s \equiv h$ ,  $r = 0$  stands for the density of energy and  $r \geq 1$  for the respective fluxes. The density of energy  $h(\mathbf{r}, t)$  follows from the trace of  $m\mathbf{I}_n^{[2]}$ , namely

$$h(\mathbf{r}, t) = \int d^3p \frac{p^2}{2m} f_1(\mathbf{r}, \mathbf{p}; t). \quad (16)$$

The set composed by  $n(\mathbf{r}, t)$ ,  $\mathbf{I}_n(\mathbf{r}, t)$ ,  $\mathbf{I}_n^{[2]}(\mathbf{r}, t)$  and  $h(\mathbf{r}, t)$  is the one corresponding to Grad's fourteen moments approach. Finally, the hydrodynamic equations are

$$\frac{\partial}{\partial t} \mathbf{I}_s^{[r]}(\mathbf{r}, t) = \int d^3p u_s^{[r]}(\mathbf{p}) \frac{\partial}{\partial t} f_1(\mathbf{r}, \mathbf{p}; t) \quad (17)$$

with  $r = 0, 1, 2, \dots$ , and where is to be introduced Eq.(27). Equations (17) consists of an enormous set of coupled nonlinear integro-differential equations. Evidently, it can be handled only in a contracted version, introducing the hydrodynamics of order 0, 1, 2, etc..., thus classified according to the last flux that is retained in the contraction of the description. Criteria for deciding the order of the contraction must be established (see Ref. [68]). Hydrodynamics of order zero leads for the density to satisfy Fick' standard diffusion equation, the one of order one to Maxwell-Cattaneo equation, and the other orders to generalized Burnett and super-Burnett equations.

To proceed further, and give a clear illustration of the functioning of the theory, we consider the case of a solution of  $N$  particles of mass  $m$  (the solute) in a fluid (the solvent) of  $N_R$  particles of mass  $M$ . The former is subjected to external forces – driving it out of equilibrium –, and the latter (the thermal bath) is taken in a steady state of constant equilibrium with an external reservoir at temperature  $T_o$ . An analogous case, but at the quantum mechanical level, is the one of carriers embedded in the ionic lattice in doped or photoinjected semiconductors (see for example [53]-[56]).

We write for the Hamiltonian

$$\hat{H} = \hat{H}_S + \hat{H}_R + \hat{W} + \hat{H}_P, \quad (18)$$

where, the first term on the right,

$$\hat{H}_S = \sum_{j=1}^N \frac{p_j^2}{2m} + \frac{1}{2} \sum_{j \neq k}^N V(|\mathbf{r}_j - \mathbf{r}_k|) \quad (19)$$

is the Hamiltonian of the particles in the solute, consisting of their kinetic energy and their pair interaction via a central force potential; the second term is

$$\hat{H}_R = \sum_{\mu=1}^{N_R} \frac{P_\mu^2}{2M} + \frac{1}{2} \sum_{\mu \neq \nu=1}^{N_R} \Phi_R(|\mathbf{R}_\mu - \mathbf{R}_\nu|) \quad (20)$$

which is the Hamiltonian of the particles in the solvent, acting as a thermal bath, consisting of their kinetic energy plus their pair in-

teraction via a central force potential; moreover

$$\hat{W} = \sum_{j=1}^N \sum_{\mu=1}^{N_R} w(|\mathbf{r}_j - \mathbf{R}_\mu|) \quad (21)$$

is the interaction Hamiltonian of the particles with the thermal bath, and  $H_P = \sum_i V_{ext}(\mathbf{r}_i, \mathbf{p}_i, t)$  is the Hamiltonian associated to the external force acting on the particles of the system.

Under the stated condition that the bath is in constant thermal equilibrium with an external reservoir at temperature  $T_o$ , its macroscopic state is characterized by the canonical distribution

$$\varrho_R = Z^{-1} \exp \left\{ -\beta_o \hat{H}_R \right\} \quad (22)$$

where  $\beta_o = [k_B T_o]^{-1}$  and  $Z$  is the corresponding partition function. The auxiliary nonequilibrium statistical operator of the whole system is the one of Eq. (3) and Eq. (4). But, for simplicity, considering a dilute solution (large distance in average between the particles) or that the potential  $V$  is screened (e.g., molecules in an ionized saline solvent, e.g. [57]), we can disregard the influence of the two particle potential, and then ignore  $\hat{n}_2$ , that is, taking  $F_2 = 0$  in Eq. (4) retaining only  $\hat{n}_1$ . In that case, we choose the single-particle reduced density,  $\hat{n}_1(\mathbf{r}, \mathbf{p} \mid \Gamma)$ , as the only relevant dynamical variable required. Hence,  $\bar{\varrho}(t, 0)$ , of Eq. (4), the aux-

iliary nonequilibrium statistical operator for the particles embedded in the bath, is

$$\begin{aligned} \bar{\varrho}(t, 0) = \exp \left\{ -\phi(t) - \int d^3r d^3p F_1(\mathbf{r}, \mathbf{p}; t) \right. \\ \left. \times \hat{n}_1(\mathbf{r}, \mathbf{p}) \right\} \\ = \prod_{j=1}^N \bar{\varrho}_j(t, 0), \end{aligned} \quad (23)$$

where

$$\begin{aligned} \bar{\varrho}_j(t, 0) = \exp \left\{ -\phi_j(t) - \int d^3r d^3p F_1(\mathbf{r}, \mathbf{p}; t) \right. \\ \left. \times \delta(\mathbf{r} - \mathbf{r}_j) \delta(\mathbf{p} - \mathbf{p}_j) \right\} \end{aligned} \quad (24)$$

is a probability distribution for an individual particle, with  $\phi(t)$  and  $\phi_j(t)$  ensuring the normalization conditions of  $\bar{\varrho}$  and  $\bar{\varrho}_j$ .

The nonequilibrium equation of state [52], that is the one relating the variables  $f_1(\mathbf{r}, \mathbf{p}; t)$  and  $F_1(\mathbf{r}, \mathbf{p}; t)$  is

$$\begin{aligned} f_1(\mathbf{r}, \mathbf{p}; t) = Tr \{ \hat{n}_1(\mathbf{r}, \mathbf{p}) \bar{\varrho}(t, 0) \} \\ = \exp \{ -F_1(\mathbf{r}, \mathbf{p}; t) \}, \end{aligned} \quad (25)$$

or

$$F_1(\mathbf{r}, \mathbf{p}; t) = -\ln f_1(\mathbf{r}, \mathbf{p}; t). \quad (26)$$

On the other hand, the evolution equation for  $f_1$  following from the NESEF-based kinetic theory, derived as shown in Ref. [58], is the generalized kinetic equation

$$\frac{\partial}{\partial t} f_1(\mathbf{r}, \mathbf{p}; t) + \frac{\mathbf{P}(\mathbf{r}, \mathbf{p}; t)}{m} \cdot \nabla f_1(\mathbf{r}, \mathbf{p}; t)$$

$$\begin{aligned}
& +\mathbf{F}(\mathbf{r}, \mathbf{p}; t) \cdot \nabla_{\mathbf{p}} f_1(\mathbf{r}, \mathbf{p}; t) - B(\mathbf{p}) f_1(\mathbf{r}, \mathbf{p}; t) \\
& - A_2^{[2]}(\mathbf{p}) \odot [\nabla_{\mathbf{p}} \nabla] f_1(\mathbf{r}, \mathbf{p}; t) \\
& - B_2^{[2]}(\mathbf{p}) \odot [\nabla_{\mathbf{p}} \nabla_{\mathbf{p}}] f_1(\mathbf{r}, \mathbf{p}; t) = 0, \quad (27)
\end{aligned}$$

obtained in the Markovian approximation [32], [34], [59], [60], where

$$\frac{\mathbf{P}(\mathbf{r}, \mathbf{p}; t)}{m} = \frac{\mathbf{p}}{m} - \mathbf{A}_1(\mathbf{p}), \quad (28)$$

$$\begin{aligned}
\mathbf{F}(\mathbf{r}, \mathbf{p}; t) &= -\nabla V_{ext}(\mathbf{r}, \mathbf{p}; t) - \mathbf{B}_1(\mathbf{p}) \\
&- \mathbf{F}_{NL}(\mathbf{r}; t), \quad (29)
\end{aligned}$$

with the explicit expressions, for the vectorial quantities  $\mathbf{A}_1(\mathbf{p})$ ,  $\mathbf{B}_1(\mathbf{p})$ ,  $\mathbf{F}_{NL}(\mathbf{r}; t)$ , the second-rank tensors  $A_2^{[2]}(\mathbf{p})$ ,  $B_2^{[2]}(\mathbf{p})$ , and the scalar  $B(\mathbf{p})$ , together with a description of the physical meaning of the several contributions, are given in Ref. [58]. We also wrote the symbol  $\odot$  for full contraction of tensors.

The distribution  $f_1(\mathbf{r}, \mathbf{p}; t)$  that follows solving Eq.(27) provides a complete information about the actual distribution of particles, and therefore of the physical properties of the system. Alternatively, if one knows all the moments of the distribution we do have a knowledge of its characteristics. A knowledge of some moments is not sufficient to determine the distribution completely; it implies in only possessing partial knowledge on the characteristics of this distribution [61] (this is related to Tchebychef's procedure for obtaining characteristics of a probability distribution when we do possess the moments

of successive order, e.g. [62]). On this H. Grad noticed that the question of the general solutions of the standard Boltzmann kinetic equation can be tackled along two distinct lines. One is to attempt to solve Boltzmann equation for the distribution  $f_1$  itself in specific problems. Other is to obtain new phenomenological equations which generalize the usual (classical-Onsagerian) fluid dynamical equations. The object is to show the transition from the Boltzmann equation in which a state is given by  $f_1(\mathbf{r}, \mathbf{p}; t)$  to the conventional fluid description in which a state is given by the density  $n(\mathbf{r}, t)$ , the velocity field  $\mathbf{v}(\mathbf{r}, t)$ , and the stress tensor  $T^{[2]}(\mathbf{r}, t)$ , in a sufficient generality to cover a broad class of problems. This approach was initiated by Maxwell [63] and continued by Grad [64] (it was called Grad's moments procedure) [65].

We do perform here an extensive generalization of the moments procedure, consisting into introducing the full set of moments of  $f_1(\mathbf{r}, \mathbf{p}; t)$ , of Eq.(27), in the variable  $\mathbf{p}$ . These moments produce quantities with a clear physical meaning, namely, the densities of particles and of energy and their fluxes of all order: the two vectorial fluxes, or currents, the tensorial fluxes, beginning with the second-order one which is the flux of the first-order flux (the current of particles) which is related to the pressure tensor, and all the other higher-order fluxes. In that way we ob-

tain a quite generalized *Mesoscopic Hydrodynamics coupled to a Non-Equilibrium Thermodynamics*, all together in the kinetic approach provided by NESEF, as described in next section.

### III. MESOSCOPIC HYDRO-THERMODYNAMICS IN NESEF.

Let us introduce, in the variable  $\mathbf{p}$ , the moments of the distribution  $f_1(\mathbf{r}, \mathbf{p}; t)$ , namely

$$n(\mathbf{r}, t) = \int d^3p f_1(\mathbf{r}, \mathbf{p}; t), \quad (30)$$

which is the density of particles;

$$\mathbf{I}_n(\mathbf{r}, t) = \int d^3p \mathbf{u}(\mathbf{p}) f_1(\mathbf{r}, \mathbf{p}; t), \quad (31)$$

where

$$\mathbf{u}(\mathbf{p}) = \mathbf{p}/m, \quad (32)$$

with  $\mathbf{I}_n$  being the flux (current) of particles;

$$I_n^{[2]}(\mathbf{r}, t) = \int d^3p \mathbf{u}^{[2]}(\mathbf{p}) f_1(\mathbf{r}, \mathbf{p}; t) \quad (33)$$

where  $\mathbf{u}^{[2]} = [\mathbf{u}\mathbf{u}]$  is the tensorial product of vectors  $\mathbf{u}$ , with  $I_n^{[2]}$  being the second-order flux (or flux of the first flux), a rank-2 tensor, which multiplied by the mass is related to the pressure tensor and

$$I_n^{[l]}(\mathbf{r}, t) = \int d^3p \mathbf{u}^{[l]}(\mathbf{p}) f_1(\mathbf{r}, \mathbf{p}; t) \quad (34)$$

are the higher-order fluxes of order  $l \geq 3$  (the previous three of Eqs. (30), (31) and (33) are those for  $l = 0, 1$  and  $2$  respectively),

where  $u^{[l]}$  is the  $l$ -rank tensor consisting of the tensorial product of  $l$  vectors  $\mathbf{u}$  of Eq. (32) that is,

$$\mathbf{u}^{[l]}(\mathbf{p}) = \left[ \frac{\mathbf{p}}{m} \frac{\mathbf{p}}{m} \dots (l - \text{times}) \dots \frac{\mathbf{p}}{m} \right]. \quad (35)$$

We do have what can be called the *family of hydrodynamical variables describing the material motion*, i. e., the set

$$\{n(\mathbf{r}, t), \mathbf{I}_n(\mathbf{r}, t), \{I_n^{[l]}(\mathbf{r}, t)\}\} \quad (36)$$

with  $l = 2, 3, \dots$

On the other hand, we have the *family of hydrodynamical variables describing the thermal motion*, consisting of

$$h(\mathbf{r}, t) = \int d^3p \frac{p^2}{2m} f_1(\mathbf{r}, \mathbf{p}; t), \quad (37)$$

$$\mathbf{I}_h(\mathbf{r}, t) = \int d^3p \frac{p^2}{2m} \frac{\mathbf{p}}{m} f_1(\mathbf{r}, \mathbf{p}; t), \quad (38)$$

$$I_h^{[l]}(\mathbf{r}, t) = \int d^3p \frac{p^2}{2m} \mathbf{u}^{[l]}(\mathbf{p}) f_1(\mathbf{r}, \mathbf{p}; t), \quad (39)$$

with  $l = 2, 3, \dots$ ; that is, in compact form those in the set

$$\{h(\mathbf{r}, t), \mathbf{I}_h(\mathbf{r}, t), \{I_h^{[l]}(\mathbf{r}, t)\}\}, \quad (40)$$

which are, respectively, the density of energy, its first vectorial flux (current), and the higher-order tensorial fluxes. It can be noticed that in this case of a parabolic type energy-momentum dispersion relation,  $E(p) = p^2/2m$ , the set of Eq. (40) is encompassed in the previous one: In fact

$$h(\mathbf{r}, t) = \frac{m}{2} \text{Tr} \{I_n^{[2]}(\mathbf{r}, t)\} \quad (41)$$

$$\mathbf{I}_h(\mathbf{r}, t) = \frac{m}{2} Tr_2 \{ I_n^{[3]}(\mathbf{r}, t) \} , \quad (42)$$

where  $Tr_2$  stands for the contraction of two indexes, and, in general

$$I_h^{[l]}(\mathbf{r}, t) = \frac{m}{2} Tr_2 \{ I_n^{[l+2]}(\mathbf{r}, t) \} , \quad (43)$$

for all the other higher-order fluxes of energy. Hence, any flux of energy of order  $l$  is contained in the flux of matter of order  $l + 2$ . In what follows we concentrate the attention on the study of the hydrodynamic motion of the particles, with heat transport to be dealt with in a future communication in this series.

#### IV. MHT EVOLUTION EQUATIONS IN NESEF

We proceed now to the derivation of the MHT equations, that is, the equations of evolutions for the basic macrovariables of the family of material motion, i. e. those in set of Eq.(36).

Let us consider the flux of order  $l$  ( $l = 0, 1, 2, \dots$ ); its evolution equation is

$$\frac{\partial}{\partial t} I_n^{[l]}(\mathbf{r}, t) = \int d^3p \, u^{[l]}(\mathbf{p}) \frac{\partial}{\partial t} f_1(\mathbf{r}, \mathbf{p}; t) . \quad (44)$$

Using Eq. (27), but excluding a dependence on  $\mathbf{p}$  of the external force, after lengthy but straightforward calculations we arrive to the general set of coupled equations for the density,  $l = 0$ , the current,  $l = 1$ , and all the other higher-order fluxes,  $l \geq 2$ , given by

$$\begin{aligned} & \frac{\partial}{\partial t} I_n^{[l]}(\mathbf{r}, t) + \nabla \cdot I_n^{[l+1]}(\mathbf{r}, t) = \\ & = \frac{1}{m} \sum_{s=1}^l \wp(1, s) [\mathcal{F}_{ext}(\mathbf{r}, t) I_n^{[l-1]}(\mathbf{r}, t)] \\ & + J_\tau^{[l]}(\mathbf{r}, t) + J_L^{[l]}(\mathbf{r}, t) + J_{NL}^{[l]}(\mathbf{r}, t), \end{aligned} \quad (45)$$

where  $\wp(1, s)$  means that we must take a permutation of the first free index (1) with the  $s$ -th ( $s=1, 2, 3, \dots, l$ ) free index of the Cartesian tensor  $[\mathcal{F}_{ext}(\mathbf{r}, t) I_n^{[l-1]}(\mathbf{r}, t)]$ , when written in the indicial notation. Observe that the number of terms in the sum is given by the number of all permutations of  $l$  symbols in which  $l - 1$  are repeated. All this ensures the correct symmetry of this contribution, that is, a fully symmetrical tensor of order  $l$ .

The several terms on the right of Eq. (45) are,

$$\mathcal{F}_{ext}(\mathbf{r}, t) = -\nabla V_{ext}(\mathbf{r}; t), \quad (46)$$

that is the applied external force, created by the action of the potential  $V_{ext}$ , and the terms  $\mathbf{A}_1(\mathbf{p})$ ,  $\mathbf{B}_1(\mathbf{p})$  and  $\mathbf{F}_{NL}(\mathbf{r}; t)$  present in Eqs. (28) and (29) have respectively been incorporated into  $J_\tau^{[l]}$ ,  $J_L^{[l]}$  and  $J_{NL}^{[l]}$ , which are,

$$\begin{aligned} J_\tau^{[l]}(\mathbf{r}, t) &= \frac{n_R}{\mathcal{V}} \frac{\sqrt{2\pi M \beta_o}}{m^2} \sum_{\mathbf{Q}} \frac{|\psi(\mathbf{Q})|^2}{Q} \times \\ & \int d^3p \sum_P [\mathbf{Q} \mathbf{Q} \mathbf{u}^{[l-2]}(\mathbf{p})] \\ & \times \exp \left[ -\alpha \left( \frac{\mathbf{Q}}{Q} \cdot \mathbf{p} \right)^2 \right] f_1(\mathbf{r}, \mathbf{p}; t) \end{aligned}$$

$$\begin{aligned}
& -\frac{n_R (M\beta_o)^{3/2} \pi}{\mathcal{V} \sqrt{2\pi m^2}} \sum_{\mathbf{Q}} \frac{|\psi(Q)|^2}{Q} \left( \frac{1}{M} + \frac{1}{m} \right) \times \\
& \int d^3 p \sum_P \left[ \mathbf{Q} \mathbf{u}^{[l-1]}(\mathbf{p}) \right] \mathbf{Q} \cdot \mathbf{p} \\
& \times \exp \left[ -\alpha \left( \frac{\mathbf{Q}}{Q} \cdot \mathbf{p} \right)^2 \right] f_1(\mathbf{r}, \mathbf{p}; t), \quad (47)
\end{aligned}$$

with  $\alpha = M\beta_o/2m^2$ ,  $\psi(Q)$  is the Fourier transform of the interaction potential between the particles and the thermal bath, i. e., Eq.(21) and according to Eq. (35)

$$\left[ \mathbf{Q} \mathbf{Q} \mathbf{u}^{[l-2]}(\mathbf{p}) \right] = \left[ \mathbf{Q} \mathbf{Q} \frac{\mathbf{p}}{m} \dots (l-2) \text{ times } \dots \frac{\mathbf{p}}{m} \right] \quad (48)$$

$$J_{NL}^{[l]}(\mathbf{r}, t) = -\frac{1}{m} \sum_{s=1}^l \wp(1, s) \left[ \mathbf{F}_{NL}(\mathbf{r}, t) I_n^{[l-1]}(\mathbf{r}, t) \right], \quad (49)$$

$$\begin{aligned}
\mathbf{F}_{NL}(\mathbf{r}; t) &= \int d^3 r' \int d^3 p' \mathbf{G}_{NL}(\mathbf{r}' - \mathbf{r}, \mathbf{p}') \\
& f_1(\mathbf{r}', \mathbf{p}'; t), \quad (50)
\end{aligned}$$

$$\mathbf{G}_{NL}(\mathbf{r}' - \mathbf{r}, \mathbf{p}') = \frac{n_R \beta_o}{\mathcal{V}} \sum_{\mathbf{Q}} \mathbf{Q} |\psi(Q)|^2$$

$$\begin{aligned}
& \times \left\{ iF(\mathbf{Q}, \mathbf{p}') \right. \\
& + \left( \frac{M\beta_o}{2\pi} \right)^{1/2} \frac{\pi}{m} \frac{\mathbf{Q} \cdot \mathbf{p}'}{Q} \times \exp \left[ -\alpha \left( \frac{\mathbf{Q}}{Q} \cdot \mathbf{p}' \right)^2 \right] \left. \right\} \\
& \times \exp \left[ i\mathbf{Q} \cdot (\mathbf{r}' - \mathbf{r}) \right], \quad (51)
\end{aligned}$$

$$\begin{aligned}
J_L^{[l]}(\mathbf{r}, t) &= -\frac{n_R M\beta_o}{\mathcal{V} m^2} \sum_{\mathbf{Q}} \frac{|\psi(Q)|^2}{Q^2} \\
& \times \mathbf{Q} \cdot \nabla \int d^3 p \sum_P \left[ \mathbf{Q} \mathbf{u}^{[l-1]}(\mathbf{p}) \right] F(\mathbf{p}, \mathbf{Q}) \\
& \times f_1(\mathbf{r}, \mathbf{p}; t), \quad (52)
\end{aligned}$$

where

$$F(\mathbf{p}, \mathbf{Q}) = 1 + \sum_{n=1}^{\infty} \frac{(-1)^n}{(2n-1)!!} 2^n \alpha^n \left( \frac{\mathbf{Q}}{Q} \cdot \mathbf{p} \right)^{2n}. \quad (53)$$

Observe that the notation

$$\begin{aligned}
& \sum_P \left[ \mathbf{Q} \mathbf{u}^{[l-1]}(\mathbf{p}) \right] \\
& \equiv \sum_P \left[ \mathbf{Q} \frac{\mathbf{p}}{m} \dots (l-1) \text{ times } \dots \frac{\mathbf{p}}{m} \right] \quad (54)
\end{aligned}$$

means that one has to sum all permutations of the vectors in order to ensure that the

tensor has the same symmetry of the tensor  $I_n^{[l]}$  on the left hand side of Eq. (45).

Next, making a Taylor series expansion of the exponential in both contributions in Eq.

(47) and in Eq. (51), i. e.,

$$\exp \left[ -\alpha \left( \frac{\mathbf{Q}}{Q} \cdot \mathbf{p} \right)^2 \right] = \sum_{k=0}^{\infty} \frac{(-1)^k \alpha^k}{k!} \mathbf{Q}^{[2k]} \odot \mathbf{p}^{[2k]}, \quad (55)$$

where  $\mathbf{Q}^{[l]}$  stands for

$$\mathbf{Q}^{[l]} = [\mathbf{Q} \dots (l - \text{times}) \dots \mathbf{Q}], \quad (56)$$

and we recall that  $\odot$  stands for full contraction of the two tensors of rank  $2k$ . Then using Eq.(53) for  $F(\mathbf{p}, \mathbf{Q})$ , we can rewrite Eqs. (47), (49) and (52) in a closed form in terms of all the fluxes, namely

$$\begin{aligned}
J_{\tau}^{[l]}(\mathbf{r}, t) &= \sum_{k=0}^{\infty} \hat{\wp}_l \left[ \Lambda_{\tau o}^{[2k+2]} \odot I_n^{[2k+l-2]}(\mathbf{r}, t) \right] \\
& + \sum_{k=0}^{\infty} \sum_{s=1}^l \wp(1, s) \left[ \Lambda_{\tau}^{[2k+2]} \odot I_n^{[2k+l]}(\mathbf{r}, t) \right], \quad (57)
\end{aligned}$$

$$J_L^{[l]}(\mathbf{r}, t) = \sum_{k=0}^{\infty} \sum_{s=1}^l \wp(1, s) \left[ \Lambda_L^{[2k+2]} \odot \nabla I_n^{[2k+l-1]}(\mathbf{r}, t) \right], \quad (58)$$

$$J_{NL}^{[l]}(\mathbf{r}, t) = -\frac{1}{m} \sum_{s=1}^l \wp(1, s) \sum_{k=0}^{\infty} \int d^3 \mathbf{r}' \left\{ \left[ \left[ \Lambda_{NL1}^{[2k+1]}(\mathbf{r}' - \mathbf{r}) \odot I_n^{[2k]}(\mathbf{r}', t) \right] I_n^{[l-1]}(\mathbf{r}, t) \right] \right. \\ \left. + \left[ \left[ \Lambda_{NL2}^{[2k+2]}(\mathbf{r}' - \mathbf{r}) \odot I_n^{[2k+1]}(\mathbf{r}', t) \right] I_n^{[l-1]}(\mathbf{r}, t) \right] \right\}, \quad (59)$$

where

$$\widehat{\wp}_l = \sum_{s=2}^l \wp(2, s) + \sum_{r=3}^l \wp(1, r) \\ + \sum_{r=3}^{l-1} \sum_{s=r+1}^l \wp(1, r; 2, s) \quad (60)$$

is an operator involving the set of permutations that ensures the proper symmetry of the tensor on which it acts. Here the operation  $\Lambda^{[r]} \odot \Lambda^{[s]}$  indicates the contraction of some indexes in order to give the right tensorial order of the equation. For example in Eqs. (57) and (58) it indicates the contraction of  $(r + s - l)/2$  indexes as to produce a tensor of rank  $l$ . The several tensorial kinetic coefficients are given in Appendix A: Eqs. (A1) to Eq. (A8).

We can see that the expressions for  $J_\tau^{[l]}$  and  $J_L^{[l]}$  are linear in the hydrodynamic basic variables of the set of Eq. (36) with tensorial coefficients  $\Lambda^{[r]}$ . The first one contains contributions of a relaxation character, and the

second involves local couplings with the different fluxes. On the other hand  $J_{NL}^{[l]}$  is non-linear (bilinear) in the fluxes accounting for nonlocal correlations involving all of them. Next, we reorganize these expressions setting into evidence the contributions that contain the neighboring fluxes to the one of order  $l$ , namely  $I_n^{[l-1]}(\mathbf{r}, t)$  and  $I_n^{[l+1]}(\mathbf{r}, t)$ , that is, arising out of the terms with  $k = 0$  and  $k = 1$  in the sum over  $k$  in Eqs. (57) and (58), to obtain Eq. (45) in the form,

$$\frac{\partial}{\partial t} I_n^{[l]}(\mathbf{r}, t) + \nabla \cdot I_n^{[l+1]}(\mathbf{r}, t) = \\ = \frac{1}{m} \sum_{s=1}^l \wp(1, s) [\mathcal{F}_{ext}(\mathbf{r}, t) I_n^{[l-1]}(\mathbf{r}, t)] \\ - \theta_l^{-1} I_n^{[l]}(\mathbf{r}, t) + a_{Lo} \sum_{s=1}^l \wp(1, s) [\nabla I_n^{[l-1]}(\mathbf{r}, t)] \\ + 2la_{L1} \nabla \cdot I_n^{[l+1]}(\mathbf{r}, t) + b_{\tau o} \left\{ \widehat{\wp}_l [\mathbf{1}^{[2]} I_n^{[l-2]}(\mathbf{r}, t)] \right\} \\ + J_{NL}^{[l]}(\mathbf{r}, t) + S_n^{[l]}(\mathbf{r}, t). \quad (61)$$

The last term on the right of Eq. (61) is given by,

$$S_n^{[l]}(\mathbf{r}, t) = b_{\tau 1} \frac{2}{m} \left\{ \widehat{\wp}_l [\mathbf{1}^{[2]} I_h^{[l-2]}(\mathbf{r}, t)] \right\} \\ + 3la_{\tau 1} \frac{2}{m} I_h^{[l]}(\mathbf{r}, t) \\ + a_{L1} \frac{2}{m} \sum_{s=1}^l \wp(1, s) [\nabla I_h^{[l-1]}(\mathbf{r}, t)] \\ + R_n^{[l]}(\mathbf{r}, t), \quad (62)$$

where  $R_n^{[l]}(\mathbf{r}, t)$ , given in Appendix A, contains the contributions of the fluxes of order

higher than  $l + 2$ ; and the kinetic coefficients  $a_{\tau 1}, a_{Lo}, a_{L1}, b_{\tau o}, b_{\tau 1}$  are given in Appendix B. The first three contributions on the right of Eq. (62) are associated to the fluxes of energy of orders  $l - 2, l - 1$  and  $l$ , terms that can be considered consisting of thermo-striction effects and which, then, couple these equations with the set of kinetic equations describing the movement of energy, i. e. the hydrodynamical variables of the set of Eq. (40). However it can be noticed the already mentioned fact that the fluxes of energy can be given in terms of those of particles, namely,  $I_h^{[l]} = (m/2)Tr_2 \left\{ I_n^{[l+2]} \right\}$ , [ cf. Eqs. (41) to (43)]. Moreover,

$$\theta_l^{-1} = l [|a_{\tau o}| + (l - 1) |b_{\tau 1}|], \quad (63)$$

with  $\theta_l$  playing the role of a Maxwell-characteristic time for the  $l$ -th flux.

We stress that  $l = 0$  corresponds to the density  $n(\mathbf{r}, t)$ ,  $l = 1$  to the first flux (current)  $\mathbf{I}_n(\mathbf{r}, t)$ ,  $l = 2$  to the second flux  $I_n^{[2]}(\mathbf{r}, t)$  which multiplied by the mass  $m$  is related to the pressure tensor  $P^{[2]}(\mathbf{r}, t)$ ,  $l > 2$  to the other higher-order fluxes. Hence, Eq. (61) represents the coupled set of evolution equations involving the density and all its fluxes in its most general form. It must be noticed that it is linear in the basic variables; no approximation has been introduced. Nonlinearities should arise out of the interparticle interaction inclusion which we have disregarded in

the present communication (case of a dilute solution). However, as already noticed, such set of equations is intractable, and, of course, we need to look in each case on how to find the best description using the smallest possible numbers of variables. In other words to introduce an appropriate – for each case – contraction of description: *this contraction implies in retaining the information considered as relevant for the problem in hands, and to disregard nonrelevant information* [67].

Elsewhere [68] we have discussed the question of the contraction of description (reduction of the dimensions of the nonequilibrium thermodynamic space of states). As shown, a criterion for justifying the different levels of contraction is derived: It depends on the range of wavelengths and frequencies which are relevant for the characterization, in terms of normal modes, of the hydrothermodynamic motion in the nonequilibrium open system. Maxwell times have a particular relevance then we proceed to analyze them.

## V. THE HIERARCHY OF MAXWELL CHARACTERISTIC TIMES

Let us now analyze Maxwell characteristics times of Eq. (63) to show that they follow a hierarchy of values. First we note that, taking into account Eq. (B7) into Eq.



(63) and the definition in Eq. (B1) we can write

$$\theta_l^{-1} = l \left[ 1 + \frac{1}{5} \frac{M}{m+M} (l-1) \right] \theta_1^{-1} \quad (64)$$

what tell us that any characteristic time for  $l \geq 2$  is proportional to the one of  $l = 1$ , that is the one for the first flux which multiplied by the mass  $m$  is the linear momentum density and then all are proportional to the linear momentum relaxation time. On the other hand we do have that

$$\frac{\theta_{l+1}}{\theta_l} = \frac{l}{l+1} \frac{5(1+x) + l - 1}{5(1+x) + l}, \quad (65)$$

for  $l = 1, 2, 3, \dots$  and where  $x = m/M$ , and then the ordering sequence

$$\theta_1 > \theta_2 > \theta_3 > \dots > \theta_l > \theta_{l+1} > \dots \quad (66)$$

is verified which can be considered to represent a kind of Bogoliubov's hierarchy of characteristic times [50] in generalized hydrodynamics, and we can see that  $\theta_l \rightarrow 0$  as  $l \rightarrow \infty$ . Moreover according to Eq. (64) it follows that

$$\theta_l = \frac{5(1+x)}{l[5(1+x) + (l-1)]} \theta_1. \quad (67)$$

Comparing with the second flux ( $l = 2$ ), the one related to the pressure tensor, it follows that for the Brownian particles ( $x \gg 1$ )  $\theta_2 \simeq \theta_1/2$  and for the Lorentz particles ( $x \ll 1$ )  $\theta_2 \simeq 5\theta_1/12$ . A comparison with

the third flux leads to the results that  $\theta_3 \simeq \theta_1/3$  and  $\theta_3 \simeq 5\theta_1/21$  for the Brownian and Lorentz particles respectively. For any  $l$  we do have approximately:

1) for the Brownian particle ( $m/M \gg 1$ )

$$\theta_l \simeq \theta_1/l, \quad (68)$$

2) for the Lorentz particle ( $m/M \ll 1$ )

$$\theta_l \simeq [5/(4+l)l] \theta_1, \quad (69)$$

or  $\theta_l \simeq 5\theta_1/l^2$  for large  $l$ .

Moreover according to Eq. (65) as the order of flux largely increases its characteristic Maxwell time approaches zero, and  $\theta_{l+1}/\theta_l \simeq 1$ , with both being practically null. In Fig. 1 it is displayed the ratio of characteristic Maxwell times, for flux of order  $\ell$  with the momentum relaxation time, as a function of  $m/M$ , i. e., the quotient of the masses  $m$  of the system and  $M$  of the thermal bath.

Figure 1: The quotient between several Maxwell characteristic times and the one of the first flux as a function of  $m/M$ .

Observe in figure-1 that the quotient of masses has little effect on  $\theta_l/\theta_1$  but it varies

significantly with the order  $\ell$  of the flux and plays a particular relevance in the criteria for establishing the contraction of description discussed below.

## VI. ON THE CRITERION OF CONTRACTED DESCRIPTION AND AN APPLICATION

Returning to the question of the contracted description it can be shown [68] that a truncation criterion can be derived, which *rests on the characteristics of the hydrodynamic motion that develops under the given experimental procedure.*

Since inclusion of higher and higher order fluxes implies in describing a motion involving increasing Knudsen numbers per hydrodynamic mode (that is governed by smaller and smaller wavelengths – larger and larger wavenumbers – accompanied by higher and higher frequencies), in a qualitative manner, we can say that, as a general “thumb rule,” the criterion indicates that *a more and more restricted contraction can be used when larger and larger are the prevalent wavelengths in the motion.* Therefore, in simpler words, when the motion becomes more and more smooth in space and time, the more reduced can be the dimension of the basic macrovariables space to be used for the description of the nonequilibrium thermodynamic state of

the system.

As shown elsewhere [68], it can be conjectured a general contraction criterion, namely, a contraction of order  $r$  (meaning keeping the densities and their fluxes up to order  $r$ ) can be introduced, once we can show that in the spectrum of wavelengths, which characterize the motion, predominate those larger than a “frontier” one,  $\lambda_{(r,r+1)}^2 = v^2 \theta_r \theta_{r+1}$ , where  $v$  is of the order of the thermal velocity and  $\theta_r$  and  $\theta_{r+1}$  the corresponding Maxwell times. We shall try to illustrate the matter using a contraction of order 2.

Let us first write down the equations of evolution, whose general expression is given in Eq. (61), corresponding to the density and its fluxes of all order, for  $\ell = 0$ : the density, for  $\ell = 1$ : the first flux of the density,  $\ell = 2$ : the flux of the first flux which multiplied by  $m$  is the pressure tensor field, and  $\ell = 3$ : the flux of the pressure. We do have, respectively,

$$\frac{\partial}{\partial t} n(\mathbf{r}, t) + \nabla \cdot \mathbf{I}_n(\mathbf{r}, t) = 0, \quad (70)$$

$$\begin{aligned} \frac{\partial}{\partial t} \mathbf{I}_n(\mathbf{r}, t) + \nabla \cdot I_n^{[2]}(\mathbf{r}, t) &= \frac{n(\mathbf{r}, t)}{m} \mathcal{F}(\mathbf{r}, t) \\ &\quad - \theta_1^{-1} \mathbf{I}_n(\mathbf{r}, t) + a_{Lo} \nabla n(\mathbf{r}, t) \\ &\quad + 2a_{L1} \nabla \cdot I_n^{[2]}(\mathbf{r}, t) + \mathbf{S}_n(\mathbf{r}, t), \end{aligned} \quad (71)$$

$$\begin{aligned} \frac{\partial}{\partial t} I_n^{[2]}(\mathbf{r}, t) + \nabla \cdot I_n^{[3]}(\mathbf{r}, t) \\ = \frac{1}{m} \{ [\mathcal{F}(\mathbf{r}, t) \mathbf{I}_n(\mathbf{r}, t)] + [\mathbf{I}_n(\mathbf{r}, t) \mathcal{F}(\mathbf{r}, t)] \} \end{aligned}$$

$$\begin{aligned}
& -\theta_2^{-1} I_n^{[2]}(\mathbf{r}, t) + a_{Lo} \{ \nabla \mathbf{I}_n(\mathbf{r}, t) + [\nabla \mathbf{I}_n(\mathbf{r}, t)]^{tr} \} \\
& + 4 a_{L1} \nabla \cdot I_n^{[3]}(\mathbf{r}, t) + b_{\tau o} n(\mathbf{r}, t) \mathbf{1}^{[2]} + S_n^{[2]}(\mathbf{r}, t), \quad (72)
\end{aligned}$$

$$\begin{aligned}
& \frac{\partial}{\partial t} I_n^{[3]}(\mathbf{r}, t) + \nabla \cdot I_n^{[4]}(\mathbf{r}, t) = \\
& \frac{1}{m} \sum_{s=1}^3 \wp(1, s) [\mathcal{F}(\mathbf{r}, t) I_n^{[2]}(\mathbf{r}, t)] \\
& - \theta_3^{-1} I_n^{[3]}(\mathbf{r}, t) \\
& + a_{Lo} \sum_{s=1}^3 \wp(1, s) [\nabla I_n^{[2]}(\mathbf{r}, t)] \\
& + 6 a_{L1} \nabla \cdot I_n^{[4]}(\mathbf{r}, t) \\
& + b_{\tau o} \{ \widehat{\wp}_3 [\mathbf{1}^{[2]} \mathbf{I}_n(\mathbf{r}, t)] \} + S_n^{[3]}(\mathbf{r}, t), \quad (73)
\end{aligned}$$

where  $\mathcal{F}(\mathbf{r}, t)$ , given in Eq. (C1), and the expressions for  $\mathbf{S}_n(\mathbf{r}, t)$ ,  $S_n^{[2]}(\mathbf{r}, t)$  and  $S_n^{[3]}(\mathbf{r}, t)$  are given in Appendix C. The Maxwell times  $\theta_1^{-1}$ ,  $\theta_2^{-1}$  and  $\theta_3^{-1}$  are obtained from Eq. (63) respectively for  $l = 1, 2$  and  $3$ . Moreover, as noticed, if we multiply Eq. (72) by the mass  $m$ , we do have an equation for the pressure field tensor

$$P^{[2]}(\mathbf{r}, t) = m I_n^{[2]}(\mathbf{r}, t), \quad (74)$$

composed of the hydrostatic contribution (the diagonal terms) and the shear stress (the non-diagonal terms) and the convective pressure (cf. Eq. (91) presented later on, but where the shear contributions have been discarded). We also mention that taking into account Eq. (88) below relating  $\mathbf{I}_n(\mathbf{r}, t)$  with the barycentric velocity  $\mathbf{v}(\mathbf{r}, t)$ , Eq. (71) can be transformed in an evolution equation

for the latter to obtain a generalized Navier-Stokes equation (future publication).

Let us now, for illustration, consider the case when we can perform a truncation in a third order, that is, to consider as basic variables  $n(\mathbf{r}, t)$  its flux  $\mathbf{I}_n(\mathbf{r}, t)$  and the pressure tensor  $m I_n^{[2]}(\mathbf{r}, t)$ . In this contracted description we consider Eqs. (70), (71) and (72) but with the further restrictions in Eqs. (71) and (72) of neglecting: **1.** the shear stress contribution, more precisely introducing the trace of the pressure tensor which is proportional to the energy density  $h(\mathbf{r}, t)$ , that is,

$$Tr \{ P^{[2]}(\mathbf{r}, t) \} = 2h(\mathbf{r}, t) \quad (75)$$

where convective pressure has been considered, cf. Eq. (89), **2.** the terms with coefficients  $a_L$  whose origin is in self-energy corrections, which simply would renormalize the kinetic coefficients, and **3.** the terms  $\mathbf{S}_n(\mathbf{r}, t)$  and  $S_n^{[2]}(\mathbf{r}, t)$  which contain the energy density  $h(\mathbf{r}, t)$  and its flux  $\mathbf{I}_h(\mathbf{r}, t)$  thus, disregarding thermo-striction effects.

The evolution equations for the chosen hydrodynamic variables,  $n(\mathbf{r}, t)$ ,  $\mathbf{I}_n(\mathbf{r}, t)$  and  $I_n^{[2]}(\mathbf{r}, t)$ , in the conditions above stated take the form

$$\frac{\partial}{\partial t} n(\mathbf{r}, t) + \nabla \cdot \mathbf{I}_n(\mathbf{r}, t) = 0, \quad (76)$$

$$\frac{\partial}{\partial t} \mathbf{I}_n(\mathbf{r}, t) + \nabla \cdot I_n^{[2]}(\mathbf{r}, t) = \frac{n(\mathbf{r}, t)}{m} \mathcal{F}(\mathbf{r}, t)$$

$$- \theta_1^{-1} \mathbf{I}_n(\mathbf{r}, t), \quad (77)$$

$$\frac{\partial}{\partial t} I_n^{[2]}(\mathbf{r}, t) + \nabla \cdot I_n^{[3]}(\mathbf{r}, t) = b_{\tau o} n(\mathbf{r}, t) \mathbf{1}^{[2]}$$

$$\begin{aligned} & -\theta_2^{-1} I_n^{[2]}(\mathbf{r}, t) \\ & + \frac{1}{m} \{ [\mathcal{F}(\mathbf{r}, t) \mathbf{I}_n(\mathbf{r}, t)] + [\mathbf{I}_n(\mathbf{r}, t) \mathcal{F}(\mathbf{r}, t)] \}. \end{aligned} \quad (78)$$

Deriving in time Eq. (76) and, next, in the result inserting  $\partial \mathbf{I}_n(\mathbf{r}, t)/\partial t$ , using Eq. (77) we arrive at the hyperbolic (Maxwell-Cattaneo type) evolution equation for  $n(\mathbf{r}, t)$

$$\begin{aligned} \frac{\partial^2}{\partial t^2} n(\mathbf{r}, t) + \frac{1}{\theta_1} \frac{\partial}{\partial t} n(\mathbf{r}, t) &= \nabla \cdot \nabla \cdot I_n^{[2]}(\mathbf{r}, t) \\ &- \nabla \cdot \left[ \frac{n(\mathbf{r}, t)}{m} \mathcal{F}(\mathbf{r}, t) \right] \end{aligned} \quad (79)$$

Furthermore, deriving in time this Eq. (79) and using Eq. (78) it follows that

$$\begin{aligned} \frac{\partial^3}{\partial t^3} n(\mathbf{r}, t) + \left[ \frac{1}{\theta_1} + \frac{1}{\theta_2} \right] \frac{\partial^2}{\partial t^2} n(\mathbf{r}, t) \\ + \frac{1}{\theta_1 \theta_2} \frac{\partial}{\partial t} n(\mathbf{r}, t) &= b_{\tau o} \nabla^2 n(\mathbf{r}, t) \\ - \nabla \cdot \nabla \cdot \nabla \cdot I_n^{[3]}(\mathbf{r}, t) &- \frac{1}{\theta_2} \nabla \cdot \left[ \frac{n(\mathbf{r}, t)}{m} \mathcal{F}(\mathbf{r}, t) \right] \\ + \frac{1}{m} \nabla \cdot \nabla \cdot \{ [\mathcal{F}(\mathbf{r}, t) \mathbf{I}_n(\mathbf{r}, t)] &+ [\mathbf{I}_n(\mathbf{r}, t) \mathcal{F}(\mathbf{r}, t)] \} \\ - \frac{\partial}{\partial t} \nabla \cdot \left[ \frac{n(\mathbf{r}, t)}{m} \mathcal{F}(\mathbf{r}, t) \right]. \end{aligned} \quad (80)$$

The divergence of the third-order flux,  $\nabla \cdot I_n^{[3]}$ , in terms of the basic variables is evaluated on the basis of Eq.(78), the evolution equation for the second-order flux, which we recall, related to the pressure tensor [cf.

Eq.(74)]. For that purpose we consider conditions such that the pressure is changing slowly in time ( $\theta_2 \partial I_n^{[2]}/\partial t \ll I_n^{[2]}$  or  $\omega \theta_2 \ll 1$  along the motion), and then from Eq.(78) follows that

$$\begin{aligned} \nabla \cdot I_n^{[3]}(\mathbf{r}, t) &= b_{\tau o} n(\mathbf{r}, t) \mathbf{1}^{[2]} \\ &- \theta_2^{-1} I_n^{[2]}(\mathbf{r}, t) \\ &+ \frac{1}{m} \{ [\mathcal{F}(\mathbf{r}, t) \mathbf{I}_n(\mathbf{r}, t)] + [\mathbf{I}_n(\mathbf{r}, t) \mathcal{F}(\mathbf{r}, t)] \}, \end{aligned} \quad (81)$$

and using this result in Eq. (80) it follows the equation

$$\begin{aligned} \frac{\partial^3}{\partial t^3} n(\mathbf{r}, t) + \left[ \frac{1}{\theta_1} + \frac{1}{\theta_2} \right] \frac{\partial^2}{\partial t^2} n(\mathbf{r}, t) \\ + \frac{1}{\theta_1 \theta_2} \frac{\partial}{\partial t} n(\mathbf{r}, t) &= \frac{1}{\theta_2} \nabla \cdot \nabla \cdot I_n^{[2]}(\mathbf{r}, t) \\ - \frac{1}{\theta_2} \nabla \cdot \left[ \frac{n(\mathbf{r}, t)}{m} \mathcal{F}(\mathbf{r}, t) \right] &- \frac{\partial}{\partial t} \nabla \cdot \left[ \frac{n(\mathbf{r}, t)}{m} \mathcal{F}(\mathbf{r}, t) \right]. \end{aligned} \quad (82)$$

To close this Eq. (82) it is necessary to evaluate  $I_n^{[2]}$  which, we recall, is given by

$$I_n^{[2]}(\mathbf{r}, t) = \int d^3 p \left[ \frac{\mathbf{p} \mathbf{p}}{m m} \right] f_1(\mathbf{r}, \mathbf{p}; t). \quad (83)$$

We resort now to the use of Eq. (25) and for  $F_1(\mathbf{r}, \mathbf{p}, t)$  we use an expansion in variable  $\mathbf{p}$ , namely

$$\begin{aligned} F_1(\mathbf{r}, \mathbf{p}, t) &= F_{1n}(\mathbf{r}, t) + \frac{\partial F_1(\mathbf{r}, \mathbf{p}, t)}{\partial \mathbf{p}} \Big|_0 \cdot \mathbf{p} \\ &+ \frac{1}{2} \frac{\partial^2 F_1(\mathbf{r}, \mathbf{p}, t)}{\partial p^2} \Big|_0 \frac{p^2}{2m} \\ &+ \frac{1}{2} \frac{\partial^2 F_1(\mathbf{r}, \mathbf{p}, t)}{\partial \mathbf{p} \partial \mathbf{p}} \Big|_0 \odot [\overset{\circ}{\mathbf{p} \mathbf{p}}] + \dots, \end{aligned} \quad (84)$$

where lower index nought indicates that the derivative is taken at  $\mathbf{p} = \mathbf{0}$ , and  $[\overset{\circ}{\mathbf{p}\mathbf{p}}]$  is the traceless part of the tensor. We rewrite  $F_1$  in the form

$$F_1(\mathbf{r}, \mathbf{p}, t) \simeq \varphi_n(\mathbf{r}, t) + \mathbf{F}_n(\mathbf{r}, t) \cdot \mathbf{p}/m + F_h(\mathbf{r}, t) \frac{p^2}{2m} \quad (85)$$

that is, keeping terms up to second order in  $\mathbf{p}$ . This is consistent with the contracted description we used, and of disregarding the shear stress, and where  $\varphi_n$ ,  $\mathbf{F}_n$  and  $F_h$  are the nonequilibrium thermodynamic variables conjugated to the density, the flux and the trace of  $I_n^{[2]}$  which is proportional to the energy. Moreover, introducing the alternative forms

$$\mathbf{F}_n(\mathbf{r}, t) \equiv -m\beta(\mathbf{r}, t)\mathbf{v}(\mathbf{r}, t), \quad (86)$$

$$F_h(\mathbf{r}, t) \equiv \beta(\mathbf{r}, t), \quad (87)$$

it follows that

$$\mathbf{I}_n(\mathbf{r}, t) = n(\mathbf{r}, t) \mathbf{v}(\mathbf{r}, t), \quad (88)$$

defining the barycentric velocity  $\mathbf{v}(\mathbf{r}, t)$ . From Eqs. (30), (31) and (33) there follows that

$$h(\mathbf{r}, t) = \frac{m}{2} \text{Tr} \{ I_n^{[2]}(\mathbf{r}, t) \} = \frac{3}{2} n(\mathbf{r}, t) \beta^{-1}(\mathbf{r}, t) + \frac{m}{2} n(\mathbf{r}, t) v^2(\mathbf{r}, t), \quad (89)$$

where we can write  $\beta^{-1}(\mathbf{r}, t) = k_B T^*(\mathbf{r}, t)$  introducing a nonequilibrium temperature

(called quasitemperature [69], [70]), as well as

$$\mathbf{I}_h(\mathbf{r}, t) = \frac{5}{2} n(\mathbf{r}, t) \beta^{-1}(\mathbf{r}, t) \mathbf{v}(\mathbf{r}, t) + \frac{m}{2} n(\mathbf{r}, t) v^2(\mathbf{r}, t) \mathbf{v}(\mathbf{r}, t), \quad (90)$$

and

$$I_n^{[2]}(\mathbf{r}, t) = \frac{1}{m} \beta^{-1}(\mathbf{r}, t) n(\mathbf{r}, t) \mathbf{1}^{[2]} + n(\mathbf{r}, t) \mathbf{v}(\mathbf{r}, t) \mathbf{v}(\mathbf{r}, t). \quad (91)$$

Introducing Eq. (91) in Eq. (82), if  $\nabla \cdot \left[ \frac{n(\mathbf{r}, t)}{m} \mathcal{F}(\mathbf{r}, t) \right] \gg \theta_2 \frac{\partial}{\partial t} \nabla \cdot \left[ \frac{n(\mathbf{r}, t)}{m} \mathcal{F}(\mathbf{r}, t) \right]$  we finally arrive at

$$\theta_1 \theta_2 \frac{\partial^3}{\partial t^3} n(\mathbf{r}, t) + [\theta_1 + \theta_2] \frac{\partial^2}{\partial t^2} n(\mathbf{r}, t) + \frac{\partial}{\partial t} n(\mathbf{r}, t) = -\nabla \cdot \mathbf{j}_n(\mathbf{r}, t), \quad (92)$$

where

$$\mathbf{j}_n(\mathbf{r}, t) = -\mathcal{D}^{[2]}(\mathbf{r}, t) \cdot \nabla n(\mathbf{r}, t) - n(\mathbf{r}, t) \mathbf{V}(\mathbf{r}, t) \quad (93)$$

plays the role of a generalized flux with at the right being present a generalized thermodynamic force, and where

$$\mathcal{D}^{[2]}(\mathbf{r}, t) = \theta_1 \left[ \frac{k_B T^*(\mathbf{r}, t)}{m} \mathbf{1}^{[2]} + [\mathbf{v}(\mathbf{r}, t) \mathbf{v}(\mathbf{r}, t)] \right] \quad (94)$$

is playing the role of a generalized diffusion tensor (composed of two parts, a first one of thermal origin and a second associated to the drift of the material) and

$$\mathbf{V}(\mathbf{r}, t) = \theta_1 \left[ \nabla \left( \frac{k_B T^*(\mathbf{r}, t)}{m} \right) \right]$$

$$+ \theta_1 \left[ \nabla \cdot [\mathbf{v}\mathbf{v}] - \frac{1}{m} \mathcal{F}(\mathbf{r}, t) \right], \quad (95) \quad [71],$$

composed of three terms, one of thermal origin another coming from the drifting movement and a third from the applied force.

Moreover, in the steady state ( $\partial n / \partial t = 0$  and then  $\mathbf{j} = 0$ ) there follows that the density satisfies the equation

$$\mathcal{D}^{[2]}(\mathbf{r}) \cdot \nabla n(\mathbf{r}) = -n(\mathbf{r}) \mathbf{V}(\mathbf{r}). \quad (96)$$

Returning to Eq.(92), its Fourier transform reads

$$\begin{aligned} i\omega [-\omega^2 \theta_1 \theta_2 - i\omega (\theta_1 + \theta_2) + 1] n(\mathbf{Q}, \omega) \\ = i\mathbf{Q} \cdot \mathbf{j}_n(\mathbf{Q}, \omega), \end{aligned} \quad (97)$$

which give us an illustration on the criterion of contraction of description: 1. In conditions such that  $\omega^2 \theta_1 \theta_2 \ll 1$ , the term with third time derivative can be neglected and the evolution equation acquires the form of a generalized hyperbolic Maxwell-Cattaneo one. 2. If further  $\omega (\theta_1 + \theta_2) \ll 1$  the second time derivative also can be neglected and we are left with a generalized parabolic diffusion-like equation, and in that way there follows a chain of increasing contractions of description of the hydrodynamic motion.

Finally, to perform numerical calculations and analyze the results we introduce a central force interaction between particles in the system with those in the bath of the Gaussian form, called the Gaussian core model (GCM)

$$w(r) = \frac{U}{\sqrt{2\pi r_o^2}} \exp \left\{ -r^2 / r_o^2 \right\}, \quad (98)$$

with the open parameters  $U$  and  $r_o$  ( $r_o$  is a length scale playing the role of a range length and  $U/r_o$  being the interaction strength). It has been noticed that this kind of potential belongs to the class of interactions which do not diverge at the origin, i.e., are bounded. They are potentials corresponding to effective interactions between the centers of mass of soft, flexible macromolecules such as polymer chains [72], dendrimers [73], and others. The centers of mass of two macromolecules can coincide without violation of the excluded volume conditions, hence implying in a bounded interaction [74]. Several studies of this potential can be consulted, for example, in Refs. [75]- [78].

It can be noticed that GCM of Eq.(98) roughly mimics a hard sphere potential with radius  $r_o$ , and that in the limit of  $r_o$  going to zero goes over a contact potential  $U \delta(r)$ . The Fourier transform is

$$\psi(\mathbf{Q}) = \frac{\pi}{\sqrt{2}} U r_o^2 \exp \left\{ -\frac{1}{4} r_o^2 Q^2 \right\}, \quad (99)$$

In terms of these results we find that

$$\theta_1^{-1} = \frac{\sqrt{\pi}}{6\sqrt{2}} \frac{n_R}{M^{1/2}} \frac{M}{m} \left( 1 + \frac{M}{m} \right) \beta_o^{3/2} U^2, \quad (100)$$

what tells us that the momentum relaxation time becomes very large for the Brownian

particle when  $m \gg M$ , and very small for the Lorentz particle when  $m \ll M$ . Furthermore, that  $\theta_1$  increases with the power  $3/2$  of the temperature  $T_o$  and, as expected, with the reciprocal of the density of scattering centers.

Moreover, it can also be noticed that in the limit of a contact potential ( $r_o \rightarrow 0$ ), the quantity

$$\frac{1}{\kappa} = \frac{\sqrt{\pi}}{2^{3/2}} \left[ 1 + \frac{m}{M} \right]^{-1} r_o \quad (101)$$

tells us that  $\kappa^{-1}$  goes to zero and then [cf. Eqs. (B4) and (B8)] the kinetic coefficients  $a_{Lo}$  and  $a_{l1}$  approach zero, i. e.  $J_L(\mathbf{r}, t)$  does not contribute.

## VII. CONCLUDING REMARKS

Briefly summarizing the results, it has been shown how a statistical nonequilibrium ensemble formalism (applicable to the study of systems even in conditions far-from equilibrium) provides a microscopic foundation for a Nonlinear Higher-Order Hydrodynamics. Its description is based on the set of hydrodynamic variables consisting of the densities of energy and matter (particles) and their fluxes of all order.

All these hydrodynamic variables are the average value over the nonequilibrium ensemble of the corresponding microscopic mechanical operators. Once the complete set

of macrovariables is given we can obtain the nonlinear hydrodynamic equations, which are the average value over the nonequilibrium ensemble of Hamilton equations of motion (in the classical level or Heisenberg equations at the quantum level) of the basic microvariables (mechanical observables). Once all these hydrodynamical variables, cf. Eqs. (30) to (34) and (37) to (39), involve the single particle distribution function  $f_1(\mathbf{r}, \mathbf{p}; t)$ , their evolution equations follow from the evolution equation for  $f_1$  [cf. Eq. (44)]. It is obtained the set of evolution equations given in Eq. (45):  $l = 0$  for the density,  $l = 1$  for the first (vectorial) flux,  $l \geq 2$  for the higher order tensorial fluxes, all of which are coupled together.

These generalized hydrodynamic equations present on the left side the conserving part of the corresponding quantity, and on the right-hand side are present the collision integrals which include the action of external sources and the contributions of scattering processes responsible for dissipative effects.

In that way we do have a quite generalized hydrodynamics under any arbitrary condition of excitation, which, as noticed, can be referred to as *Mesoscopic Hydro-Thermodynamics*.

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## Appendix A: Tensorial Coefficients of Eqs. (57)-(59) and Last Term in Eq. (62)

The kinetic tensorial coefficients of Eq. (57) to Eq. (59) are:

$$\Lambda_{\tau o}^{[2k+2]} = \sum_{\mathbf{Q}} g_{\tau k}(Q) \mathbf{Q}^{[2k+2]}, \quad (\text{A1})$$

$$\Lambda_{\tau}^{[2k+2]} = \sum_{\mathbf{Q}} f_{\tau k}(Q) \mathbf{Q}^{[2k+2]}, \quad (\text{A2})$$

$$\Lambda_L^{[2k+2]} = \sum_{\mathbf{Q}} f_{Lk}(Q) \mathbf{Q}^{[2k+2]}, \quad (\text{A3})$$

$$\begin{aligned} \Lambda_{NL1}^{[2k+1]}(\mathbf{r}' - \mathbf{r}) &= i \frac{n_R \beta_o}{\mathcal{V}} \sum_{\mathbf{Q}} |\psi(Q)|^2 e^{i\mathbf{Q} \cdot (\mathbf{r}' - \mathbf{r})} \\ &\times \frac{(-1)^k}{(2k-1)!!} \left( \frac{M\beta_o}{Q^2} \right)^k \mathbf{Q}^{[2k+1]}, \end{aligned} \quad (\text{A4})$$

$$\Lambda_{NL2}^{[2k+2]}(\mathbf{r}' - \mathbf{r}) = \frac{n_R \beta_o (M\beta_o)^{1/2} \pi}{\mathcal{V} \sqrt{2\pi}} \times \sum_{\mathbf{Q}} \frac{|\psi(Q)|^2}{Q} e^{i\mathbf{Q} \cdot (\mathbf{r}' - \mathbf{r})} \frac{(-1)^k}{k!} \left( \frac{M\beta_o}{2Q^2} \right)^k \mathbf{Q}^{[2k+2]}.$$

(A5)

Where we have defined,

$$g_{\tau k}(Q) = \frac{n_R \sqrt{2\pi M\beta_o}}{\mathcal{V} m^2} \frac{|\psi(Q)|^2}{Q} \frac{(-1)^k}{k!} \left( \frac{M\beta_o}{2Q^2} \right)^k, \quad (\text{A6})$$

$$\begin{aligned} f_{\tau k}(Q) &= \frac{n_R (M\beta_o)^{3/2} \pi}{\mathcal{V} \sqrt{2\pi} m} \frac{|\psi(Q)|^2}{Q} \left( \frac{1}{M} + \frac{1}{m} \right) \\ &\frac{(-1)^{k+1}}{k!} \left( \frac{M\beta_o}{2Q^2} \right)^k, \end{aligned} \quad (\text{A7})$$

$$f_{Lk}(Q) = \frac{n_R M\beta_o}{\mathcal{V} m^2} \frac{|\psi(Q)|^2}{Q^2} \frac{(-1)^{k+1}}{(2k-1)!!} \left( \frac{M\beta_o}{Q^2} \right)^k. \quad (\text{A8})$$

The last term on the right of Eq. (62) is given by,

$$R_n^{[l]}(\mathbf{r}, t) = J_{\tau R}^{[l]}(\mathbf{r}, t) + J_{LR}^{[l]}(\mathbf{r}, t), \quad (\text{A9})$$

$$\begin{aligned} J_{LR}^{[l]}(\mathbf{r}, t) &= \sum_{k=2}^{\infty} \sum_{s=1}^l \wp(1, s) \left[ \Lambda_L^{[2k+2]} \right. \\ &\left. \odot \nabla I_n^{[2k+l-1]}(\mathbf{r}, t) \right], \end{aligned} \quad (\text{A10})$$

$$\begin{aligned} J_{\tau R}^{[l]}(\mathbf{r}, t) &= \sum_{k=2}^{\infty} \sum_{s=1}^l \wp(1, s) \left[ \Lambda_{\tau}^{[2k+2]} \odot I_n^{[2k+l]}(\mathbf{r}, t) \right] \\ &+ \sum_{k=2}^{\infty} \left\{ \widehat{\wp}_l \left[ \Lambda_{\tau o}^{[2k+2]} \odot I_n^{[2k+l-2]}(\mathbf{r}, t) \right] \right\}, \end{aligned} \quad (\text{A11})$$

where the operators  $\wp(1, s)$  and  $\widehat{\wp}_l$  are defined in the main text.



**Appendix B: The Kinetic Coefficients**  
in Eqs. (61) and (62)

We do have that,

$$a_{\tau o} = \frac{\mathcal{V}}{(2\pi)^3} \frac{4\pi}{3} \int dQ Q^4 f_{\tau o}(Q) \quad (\text{B1})$$

with  $k = 0$  in Eq. (11). And

$$f_{\tau o}(Q) = -\frac{n_R}{\mathcal{V}} \frac{(M\beta_o)^{3/2} \pi |\psi(Q)|^2}{\sqrt{2\pi} m^2} \frac{1}{Q} \left( \frac{m}{M} + 1 \right) \quad (\text{B2})$$

where  $\psi(Q)$  is the Fourier transform of the potential energy  $w(|\mathbf{r}_j - \mathbf{R}_\mu|)$ ,  $n_R$  is the density of particles in the thermal bath,  $\mathcal{V}$  is the volume, and  $\beta_o^{-1} = k_B T_o$ . Moreover,

$$a_{\tau 1} = -\frac{M\beta_o}{10} a_{\tau o}, \quad (\text{B3})$$

$$a_{L o} = \sqrt{\frac{2}{M\beta_o \pi}} \frac{1}{\kappa} a_{\tau o}, \quad (\text{B4})$$

$$\frac{1}{\kappa} = \frac{\int dQ Q^2 |\psi(Q)|^2}{\int dQ Q^3 |\psi(Q)|^2 \left(1 + \frac{m}{M}\right)}, \quad (\text{B5})$$

$$b_{\tau o} = -\frac{2}{M\beta_o} a_{\tau o} \left(1 + \frac{m}{M}\right)^{-1}, \quad (\text{B6})$$

$$b_{\tau 1} = \frac{a_{\tau o}}{5} \left(1 + \frac{m}{M}\right)^{-1}, \quad (\text{B7})$$

$$a_{L 1} = -\frac{1}{5\kappa} \sqrt{\frac{2M\beta_o}{\pi}} a_{\tau o}. \quad (\text{B8})$$

**Appendix C: The Last Terms of Eqs. (71), (72) and (73)**

The contributions present in Eqs. (71), (72) and (73) in section VI are

$$\mathcal{F}(\mathbf{r}, t) = -\nabla V_{ext}(\mathbf{r}; t) - \mathbf{F}_{NL}(\mathbf{r}; t), \quad (\text{C1})$$

$$\mathbf{S}_n(\mathbf{r}, t) = 3a_{\tau 1} \frac{2}{m} \mathbf{I}_h(\mathbf{r}, t) + \frac{2}{m} a_{L 1} \nabla h(\mathbf{r}, t)$$

$$+ \mathbf{R}_n(\mathbf{r}, t), \quad (\text{C2})$$

$$\begin{aligned} S_n^{[2]}(\mathbf{r}, t) &= \frac{2}{m} b_{\tau 1} h(\mathbf{r}, t) \mathbf{1}^{[2]} + 6a_{\tau 1} \frac{2}{m} I_h^{[2]}(\mathbf{r}, t) \\ &+ a_{L 1} \frac{2}{m} \{ \nabla \mathbf{I}_h(\mathbf{r}, t) + [\nabla \mathbf{I}_h(\mathbf{r}, t)]^{tr} \} + R_n^{[2]}(\mathbf{r}, t), \end{aligned} \quad (\text{C3})$$

where upper index  $tr$  stands for transpose,

$$\begin{aligned} S_n^{[3]}(\mathbf{r}, t) &= b_{\tau 1} \frac{2}{m} \{ \widehat{\wp}_3 [\mathbf{1}^{[2]} \mathbf{I}_h(\mathbf{r}, t)] \} \\ &+ a_{L 1} \frac{2}{m} \sum_{s=1}^3 \wp(1, s) [\nabla I_h^{[2]}(\mathbf{r}, t)] \\ &+ 9a_{\tau 1} \frac{2}{m} I_h^{[3]}(\mathbf{r}, t) + R_n^{[3]}(\mathbf{r}, t). \end{aligned} \quad (\text{C4})$$

In which,

$$\begin{aligned} \mathbf{R}_n(\mathbf{r}, t) &= \sum_{k=2}^{\infty} \{ \Lambda_{\tau}^{[2k+2]} \odot I_n^{[2k+1]}(\mathbf{r}, t) \\ &+ \Lambda_L^{[2k+2]} \odot \nabla I_n^{[2k]}(\mathbf{r}, t) \}, \end{aligned} \quad (\text{C5})$$

$$R_n^{[2]}(\mathbf{r}, t) = \sum_{k=2}^{\infty} \{ \Lambda_{\tau o}^{[2k+2]} \odot I_n^{[2k]}(\mathbf{r}, t)$$

$$+ \Lambda_{\tau}^{[2k+2]} \odot I_n^{[2k+2]}(\mathbf{r}, t)$$

$$\begin{aligned} &+ I_n^{[2k+2]}(\mathbf{r}, t) \odot \Lambda_{\tau}^{[2k+2]} + \Lambda_L^{[2k+2]} \odot \nabla I_n^{[2k+1]}(\mathbf{r}, t) \\ &+ \left[ \Lambda_L^{[2k+2]} \odot \nabla I_n^{[2k+1]}(\mathbf{r}, t) \right]^{tr} \}, \end{aligned} \quad (\text{C6})$$

$$R_n^{[3]}(\mathbf{r}, t) = J_{\tau R}^{[3]}(\mathbf{r}, t) + J_{LR}^{[3]}(\mathbf{r}, t), \quad (\text{C7})$$

$$\begin{aligned}
J_{LR}^{[3]}(r, t) &= \sum_{k=2}^{\infty} \sum_{s=1}^3 \wp(1, s) \left[ \Lambda_L^{[2k+2]} \odot \nabla I_n^{[2k+2]}(\mathbf{r}, t) \right], \\
&+ \sum_{k=2}^{\infty} \sum_{s=1}^3 \wp(1, s) \left[ \Lambda_{\tau}^{[2k+2]} \odot I_n^{[2k+3]}(\mathbf{r}, t) \right].
\end{aligned} \tag{C8}$$

The several kinetic tensorial coefficients  $\Lambda^{[r]}$  are given in Appendix A.

$$J_{\tau R}^{[3]}(\mathbf{r}, t) = \sum_{k=2}^{\infty} \widehat{\wp}_3 \left[ \Lambda_{\tau o}^{[2k+2]} \odot I_n^{[2k+1]}(\mathbf{r}, t) \right],$$

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